

On-surface synthesis of graphene nanoribbons from a computational perspective

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Graphene nanoribbons (GNRs) are strips of graphene with nanoscale widths, meaning widths below 100 nm. Besides the width limit, the term GNR imposes no hard geometrical constraints in terms of length, aspect ratio or edge shape, and thus applies to a diverse set of graphene-derived nanostructures. Atomically precise GNRs promise to combine the outstanding electronic properties of graphene with an electronic band gap that is sufficiently large for digital-logic applications at room temperature.

It has been shown that atomically precise GNRs can be fabricated by an on-surface synthesis approach [1]. This versatile method has been successfully applied to the fabrication of armchair GNRs (AGNRs) of different widths -and thus different band gaps- as well as more complicated structures like chevron GNRs or heterojunctions [2]. More recently, it has also been extended to afford the fabrication of GNRs with zigzag edges (ZGNRs) [3], which are predicted to exhibit spin-polarized edge states

I will briefly review the on-surface synthesis approach to AGNRs from a simulation point of view, and discuss some recent additions to the family of GNRs such as atomically precise 6-ZGNRs [3]. I will then focus on the present challenges that simulations encounter in characterizing nanographenes on metallic substrates [4, 5] when they have to compare to experiments. Finally, I will discuss a family of zigzag edge-extended AGNRs hosting topological electronic phases. It will be shown that variations of the AGNR backbone width and the zigzag edge segment spacing drive this family of GNR structures into trivial, metallic and topological insulating phases [6].

[1] J. Cai et al., *Nature* **466**, 470 (2010).

[2] L.Talirz et al., *Adv. Mater.* **28**, 6222 (2016).

[3] P. Ruffieux et al., *Nature* **531**, 489 (2016).

[4] J.I. Urgel et al., *J. Am. Chem. Soc.* **139**, 11658 (2017).

[5] J.Wilhelm et al., *J. Phys. Chem. Lett.* **9**, 306 (2018).

[6] O. Gröning et al., *Nature* **560**, 209 (2018).